Yoyo Hinuma

List of Publications by Year
in descending order

25 papers	1,280 citations	567144 15 h-index	610775 24 g-index
25 all docs	25 docs citations	25 times ranked	1903 citing authors

#	Article	IF	Citations
1	Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184.	1.4	457
2	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. Physical Review B, 2014, 90, .	1.1	271
3	Density Functional Theory Calculations of Oxygen Vacancy Formation and Subsequent Molecular Adsorption on Oxide Surfaces. Journal of Physical Chemistry C, 2018, 122, 29435-29444.	1.5	103
4	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. Physical Review B, 2017, 96, .	1.1	85
5	Band offsets of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/CdS and CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/ZnS (110) interfaces: A hybrid density functional theory study. Physical Review B, 2013, 88, .	1.1	50
6	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
7	Band alignment at surfaces and heterointerfaces of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>, and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2019, 3, .	0.9	32
8	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	24
9	Linear Correlations between Adsorption Energies and HOMO Levels for the Adsorption of Small Molecules on TiO₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 20988-20997.	1.5	23
10	Changes in Surface Oxygen Vacancy Formation Energy at Metal/Oxide Perimeter Sites: A Systematic Study on Metal Nanoparticles Deposited on an In₂O₃(111) Support. Journal of Physical Chemistry C, 2020, 124, 27621-27630.	1.5	22
11	Frontier Molecular Orbital Based Analysis of Solidâ€“Adsorbate Interactions over Group 13 Metal Oxide Surfaces. Journal of Physical Chemistry C, 2020, 124, 15355-15365.	1.5	22
12	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. Journal of Applied Physics, 2019, 125, .	1.1	19
13	Surface Oxygen Vacancy Formation Energy Calculations in 34 Orientations of Î²-Ga₂O₃ and Î¸-Al₂O₃. Journal of Physical Chemistry C, 2020, 124, 10509-10522.	1.5	19
14	Effect of Oxygen Vacancies on Adsorption of Small Molecules on Anatase and Rutile TiO₂ Surfaces: A Frontier Orbital Approach. Journal of Physical Chemistry C, 2021, 125, 3827-3844.	1.5	18
15	Reaction Mechanism of Li₂MnO₃ Electrodes in an All-Solid-State Thin-Film Battery Analyzed by Operando Hard X-ray Photoelectron Spectroscopy. Journal of the American Chemical Society, 2022, 144, 236-247.	6.6	16
16	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. Physical Review B, 2013, 88, .	1.1	15
17	The effect of cation size on hydride-ion conduction in LnSrLiH₂O₂ (Ln = La,) Tj ETQq1 1 0.784314 rgBT /Ov	5.2	15
18	Reactions of the Li₂MnO₃ Cathode in an All-Solid-State Thin-Film Battery during Cycling. ACS Applied Materials & Interfaces, 2021, 13, 7650-7663.	4.0	13

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19	Factors determining surface oxygen vacancy formation energy in ternary spinel structure oxides with zinc. Physical Chemistry Chemical Physics, 2021, 23, 23768-23777.	1.3	12
20	Surface activation by electron scavenger metal nanorod adsorption on TiH₂, TiC, TiN, and Ti₂O₃. Physical Chemistry Chemical Physics, 2021, 23, 16577-16593.	1.3	9
21	Experimental and Theoretical Investigation of Metalâ€“Support Interactions in Metal-Oxide-Supported Rhenium Materials. Journal of Physical Chemistry C, 2022, 126, 4472-4482.	1.5	5
22	A simplified methodology for the modeling of interfaces of elementary metals. AIP Advances, 2021, 11, .	0.6	3
23	Understanding and controlling the formation of surface anion vacancies for catalytic applications. Catalysis Science and Technology, 2022, 12, 2398-2410.	2.1	2
24	Trends in Surface Oxygen Formation Energy in Perovskite Oxides. ACS Omega, 2022, 7, 18427-18433.	1.6	2
25	Categorization of inorganic crystal structures by Delaunay tetrahedralization. Science and Technology of Advanced Materials Methods, 2022, 2, 75-83.	0.4	0